

## Acknowledgements

## **The Probabilistic Computing Project:**



Standing Row (L to R): Feras Saad, Marco Cusumano-Towner, Jonathan Rees, Sara Rendtorff-Smith, Josh Thayer, Zane Shelby, Ulrich Schaechtle

Seated Row (L to R): Vikash Mansinghka, Amanda Brower, Desiree Dudley, Cameron Freer, Alex Lew, Tim Trautman

## With the fiscal support of:





## **Outline**



1. Motivation

2. What is probabilistic programming?

Pedagogical example: simple (or not-so-simple) curve fitting

3. Programmable inference, not just black-box

Application: machine perception via inverse graphics

4. Learning the structure and parameters of probabilistic programs

Application: automatic data modeling for scientific data analysis

5. The MIT Modeling and Inference Stack

## **Exuberance about machine learning and "big data"**

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**WIRED MAGAZINE: 16.07** 

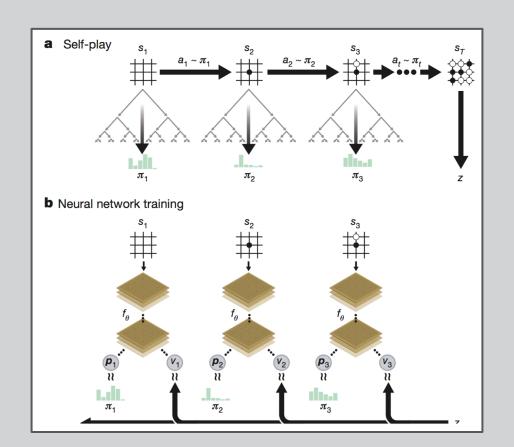
SCIENCE : DISCOVERIES

The End of Theory: The Data Deluge Makes the Scientific Method Obsolete

By Chris Anderson 🔀

06.23.08

## Machine learning success story: AlphaGo Zero



## The limitations of machine learning

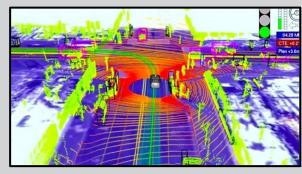
#### Go



same rules for ~2,500 years

one winner, one loser

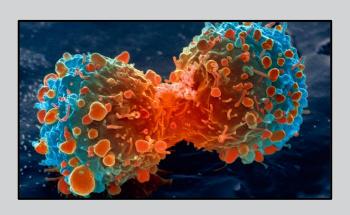
# Autonomous driving



simulations are available, but environment varies widely

drivers and pedestrians have complex & conflicting objectives

#### Cancer



every cancer cell is different

treatment requires life-and-death tradeoffs

## Challenge #1: Machine common-sense, at the level of an 18-month-old

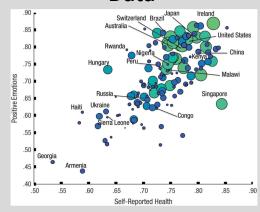


# Challenge #2: Machine expert systems that help human experts collaboratively interpret empirical data





#### **Data**



#### **Prior knowledge from:**

- Epidemiologists
- Economists
- Field workers
- Policy advocates
- Stakeholders

## What we need

Intelligence is not just about pattern recognition.

## It is about *modeling the world*...

- o explaining and understanding what we see.
- o imagining things we could see but haven't yet.
- o making judgment calls in ambiguous situations.
- o problem solving and planning actions to make these things real.
- o building new models as we learn more about the world.
- o sharing our models with each other, via language.

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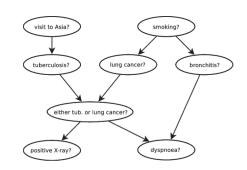
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4. Learning the structure and parameters of probabilistic programs

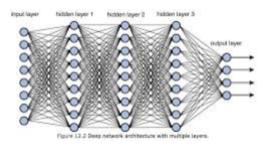
Application: automatic data modeling for scientific data analysis

5. The MIT Modeling and Inference Stack

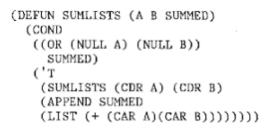
## The need for probabilistic programming



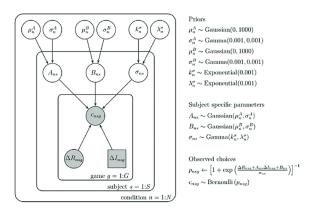
Causal models



Deep neural networks



#### Symbolic programs



**Hierarchical Bayesian models** 

## What is probabilistic programming?

#### Two technical ideas:

- 1. Models can be represented using programs that make stochastic choices
- 2. Operations on models can be represented as meta-programs

## What is probabilistic programming?

#### Two technical ideas:

- 1. Models can be represented using programs that make stochastic choices
- 2. Operations on models can be represented as meta-programs

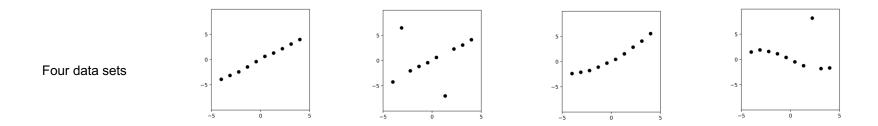
**Inference** - finding probable values for latent variables

**Learning** - finding probable model parameters and structure models given data

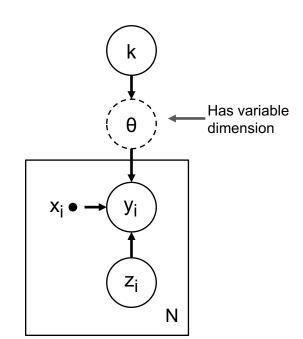
Querying - making predictions for previously unseen data, given a model

**Analysis** - estimating the amount of information between variables in a model

#### Curve fitting with model selection and outlier detection



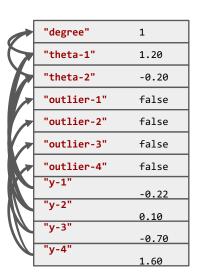
 $k \sim \operatorname{Uniform}(\{1,2,3,4\}) \qquad \qquad /\!/ \text{ Choose degree of polynomial } \\ \boldsymbol{\theta} \sim \operatorname{Normal}(\mathbf{0}_{k+1},\mathbf{I}_{k+1}) \qquad /\!/ \text{ Choose coefficients } \\ z_i \sim \operatorname{Bernoulli}(0.1) \text{ for } i=1\dots N \qquad /\!/ \text{ Choose outlier assignments } \\ y_i \sim \left\{ \begin{array}{ll} \operatorname{Normal}(\sum_{j=1}^{k+1} x_i^{j-1}\theta_j,1) & \text{if } z_i=0 \\ \operatorname{Normal}(\sum_{i=1}^{k+1} x_i^{j-1}\theta_j,10) & \text{if } z_i=1 \end{array} \right. \text{ for } i=1\dots N \\ \end{array}$ 



As a graphical model

```
@probabilistic function model(x::Vector{Float64})
    # prior over degree of polynomial
    degree prior = [0.25, 0.25, 0.25, 0.25]
    # generate degree (either 1, 2, 3, or 4)
    degree = @choice(categorical(degree prior), "degree")
    # generate parameters
    parameters = Vector{Float64}(degree+1)
    for k=1:(degree+1)
        parameters[k] = @choice(normal(prior mean, prior std), "theta-$k")
    end
    # generate data
    y = Vector{Float64}(length(x))
    for i=1:length(x)
       if degree == 1
            y_mean = dot(parameters, [1., x[i]])
        elseif degree == 2
            y_mean = dot(parameters, [1., x[i], x[i]^2])
        elseif degree == 3
            y_mean = dot(parameters, [1., x[i], x[i]^2, x[i]^3])
        else
            y mean = dot(parameters, [1., x[i], x[i]^2, x[i]^3, x[i]^4])
        end
        is outlier = @choice(flip(prob outlier), "outlier-$i")
       noise = is outlier ? outlier noise : inlier noise
       y[i] = @choice(normal(y_mean, noise), "y-$i")
    end
end
```

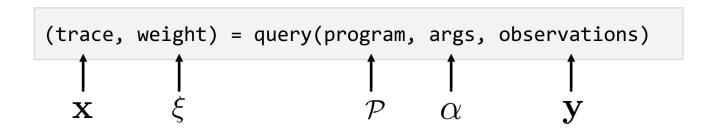
As a probabilistic program



## One possible **execution trace** of the program

with input x = [-3, 0, 2, 3]and output y = [-0.22, 0.1, -0.70, 1.60]

#### Inference in a probabilistic program



Distribution on traces induced by executing program (e.g. the prior)

Distribution on traces conditioned on observations (e.g. the posterior)

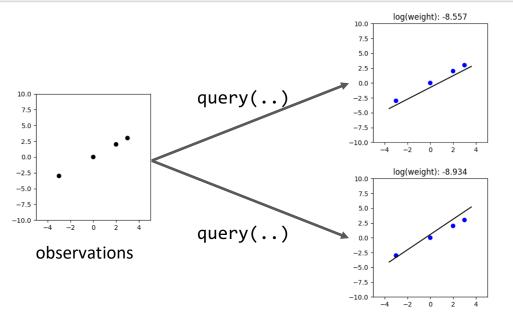
 $p(\mathbf{x}|\mathbf{y}; \mathcal{P}, \alpha) \propto p(\mathbf{x}; \mathcal{P}, \alpha) \prod_{i \in \mathbf{y}} \delta(x_i, y_i)$ 

Distribution on traces sampled during query execution  $q(\mathbf{x}; \mathcal{P}, \alpha, \mathbf{y}) \approx p(\mathbf{x}|\mathbf{y}; \mathcal{P}, \alpha)$  (e.g. the posterior approximation)

 $p(\mathbf{x}; \mathcal{P}, \alpha)$ 

#### Querying a probabilistic program

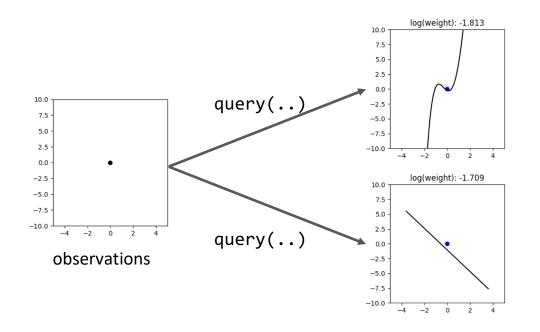
```
observations = Trace()
observations["y-1"] = -3.0
observations["y-2"] = 0.0
observations["y-3"] = 2.0
observations["y-4"] = 3.0
(trace, weight) = query(model, ([-3, 0, 2, 3],), observations)
```

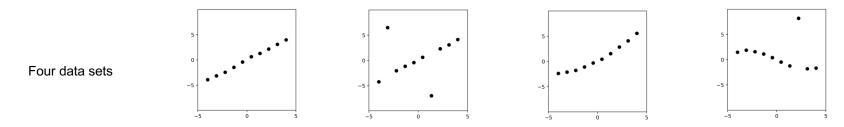


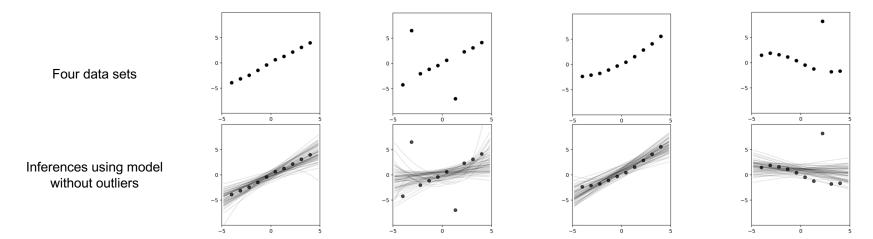
#### Querying a probabilistic program

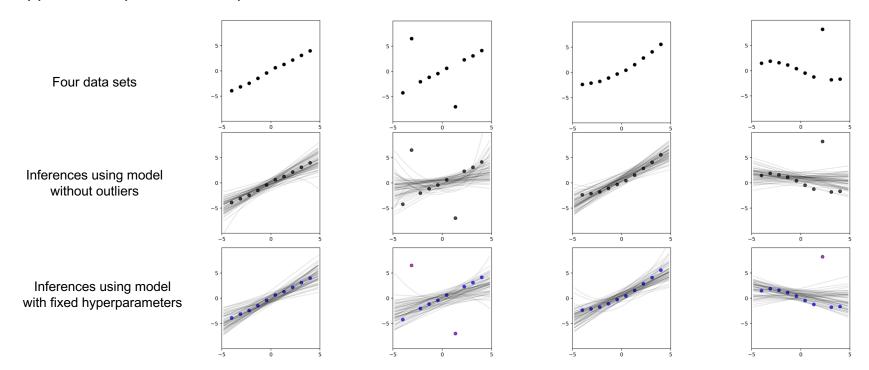
#### Observing a single data point

```
observations = Trace()
observations["y-2"] = 0.0
(trace, weight) = query(model, ([-3, 0, 2, 3],), observations)
```







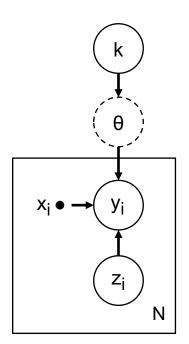


$$k \sim \text{Uniform}(\{1, 2, 3, 4\})$$

$$\boldsymbol{\theta} \sim \text{Normal}(\mathbf{0}_{k+1}, \mathbf{I}_{k+1})$$

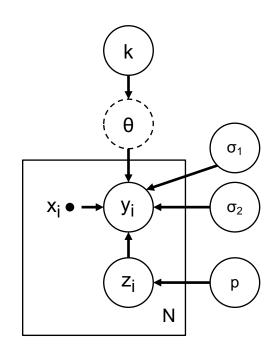
$$z_i \sim \text{Bernoulli}(0.1) \text{ for } i = 1 \dots N$$

$$y_i \sim \begin{cases} \text{Normal}(\sum_{j=1}^{k+1} x_i^{j-1} \theta_j, 1) & \text{if } z_i = 0 \\ \text{Normal}(\sum_{j=1}^{k+1} x_i^{j-1} \theta_j, 10) & \text{if } z_i = 1 \end{cases} \text{ for } i = 1 \dots N$$



Model with fixed hyperparameters

```
k \sim \text{Uniform}(\{1, 2, 3, 4\})
\boldsymbol{\theta} \sim \text{Normal}(\mathbf{0}_{k+1}, \mathbf{I}_{k+1})
p \sim \text{Beta}(1, 20)
\sigma_1 \sim \text{Gamma}(2, 1)
\sigma_2 \sim \text{Gamma}(1, 20)
z_i \sim \text{Bernoulli}(p) \text{ for } i = 1 \dots N
y_i \sim \begin{cases} \text{Normal}(\sum_{j=1}^{k+1} x_i^{j-1} \theta_j, \sigma_1) & \text{if } z_i = 0 \\ \text{Normal}(\sum_{j=1}^{k+1} x_i^{j-1} \theta_j, \sigma_2) & \text{if } z_i = 1 \end{cases} \text{ for } i = 1 \dots N
```



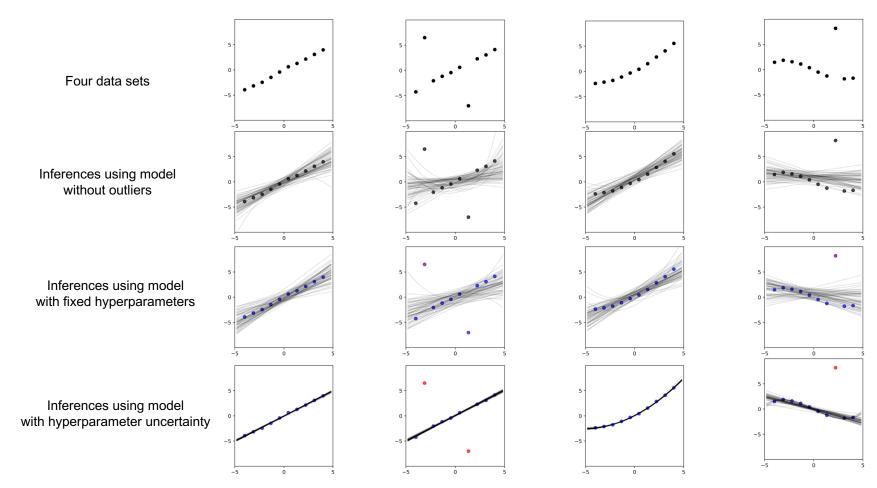
Model with hyperparameter uncertainty

```
@probabilistic function model(x::Vector{Float64})
    # prior over degree of polynomial
    degree_prior = [0.25, 0.25, 0.25, 0.25]
    # generate degree (either 1, 2, 3, or 4)
    degree = @choice(categorical(degree prior), "degree")
    # generate parameters
    parameters = Vector{Float64}(degree+1)
    for k=1:(degree+1)
        parameters[k] = @choice(normal(0, 1), "theta-$k")
    end
    # generate data
    y = Vector{Float64}(length(x))
    for i=1:length(x)
        if degree == 1
            y_mean = dot(parameters, [1., x[i]])
        elseif degree == 2
            y_{mean} = dot(parameters, [1., x[i], x[i]^2])
        elseif degree == 3
            y_mean = dot(parameters, [1., x[i], x[i]^2, x[i]^3])
        else
            y_mean = dot(parameters, [1., x[i], x[i]^2, x[i]^3, x[i]^4])
        end
        is outlier = @choice(flip(0.1), "outlier-$i")
        noise = is_outlier ? 10.0 : 1.0
        y[i] = @choice(normal(y_mean, noise), "y-$i")
    end
end
```

Model with fixed hyperparameters

```
@probabilistic function model(x::Vector{Float64})
    # prior over degree of polynomial
    degree prior = [0.25, 0.25, 0.25, 0.25]
    # generate degree (either 1, 2, 3, or 4)
    degree = @choice(categorical(degree prior), "degree")
    # generate parameters
    parameters = Vector{Float64}(degree+1)
    for k=1:(degree+1)
        parameters[k] = @choice(normal(0, 1), "theta-$k")
    end
    # hyperparameters
    inlier noise = @choice(gamma(2., 1.), "inlier-noise")
    outlier noise = @choice(gamma(10., 1.), "outlier-noise")
    prob_outlier = @choice(beta(1., 20.), "prob-outlier")
    # generate data
    y = Vector{Float64}(length(x))
    for i=1:length(x)
        if degree == 1
            y_mean = dot(parameters, [1., x[i]])
        elseif degree == 2
            y_{mean} = dot(parameters, [1., x[i], x[i]^2])
        elseif degree == 3
            y_mean = dot(parameters, [1., x[i], x[i]^2, x[i]^3])
        else
            y_mean = dot(parameters, [1., x[i], x[i]^2, x[i]^3, x[i]^4])
        end
        is outlier = @choice(flip(prob outlier), "outlier-$i")
        noise = is_outlier ? outlier_noise : inlier_noise
        y[i] = @choice(normal(y_mean, noise), "y-$i")
    end
end
```

Model with hyperparameter uncertainty



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Application: machine perception via inverse graphics

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## Probabilistic models and inference algorithms

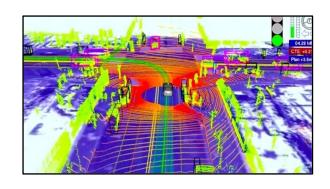
## **Statistics**

# P<sub>2,5</sub> P<sub>2,4</sub> P<sub>2,3</sub> P<sub>2,2</sub> P<sub>2,1</sub> P<sub>1,5</sub> P<sub>1,4</sub> P<sub>1,3</sub> P<sub>1,2</sub> P<sub>1,1</sub> 0.1 0.2 0.3 0.4 0.5 0.6 0.7 estimate (probability)

Model: numerical effect sizes

**Algorithm:** Markov chain Monte Carlo inference to quantify uncertainty

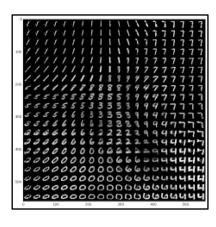
## **Robotics**



Model: tracks of vehicle & people

**Algorithm:** Particle filter to track small changes over time

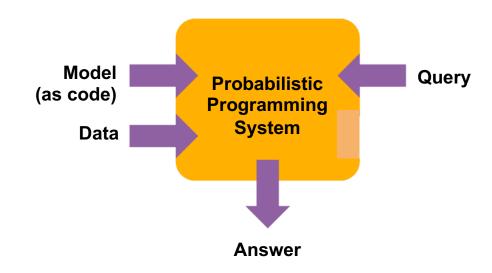
# Machine learning



**Model:** neural network parameters

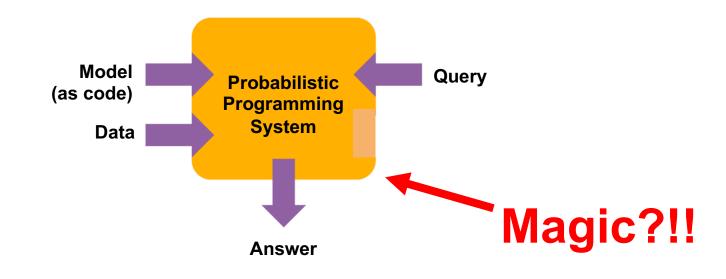
**Algorithm:** ``best" parameters found by stochastic gradient descent

## **Probabilistic programming**



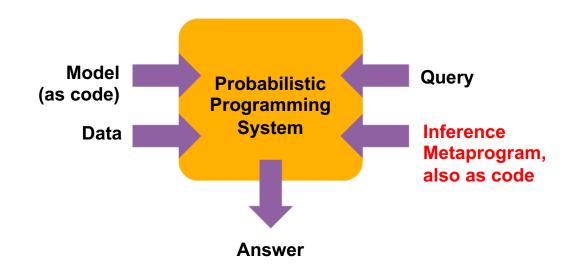
See e.g. Church, published in Goodman\*, Mansinghka\*, et al. (2008)

## Probabilistic programming with programmable inference

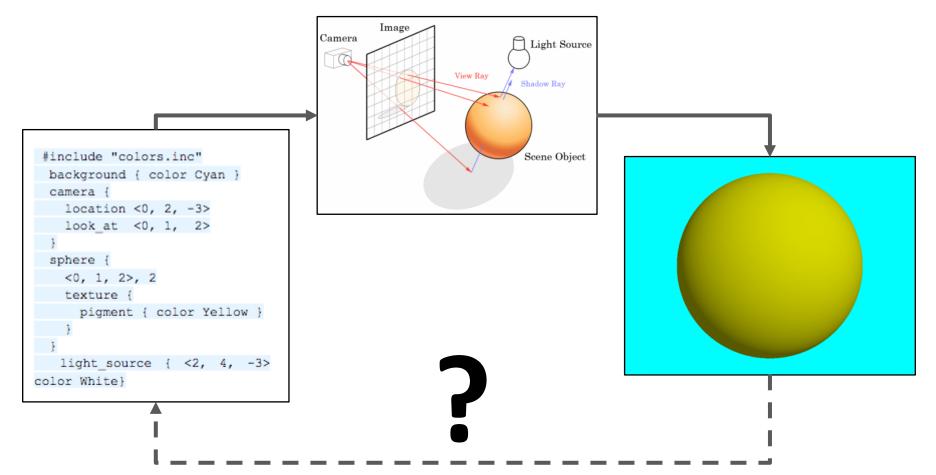


See e.g. Church (Goodman\*, Mansinghka\*, et al. [2008]), Prolog, ...

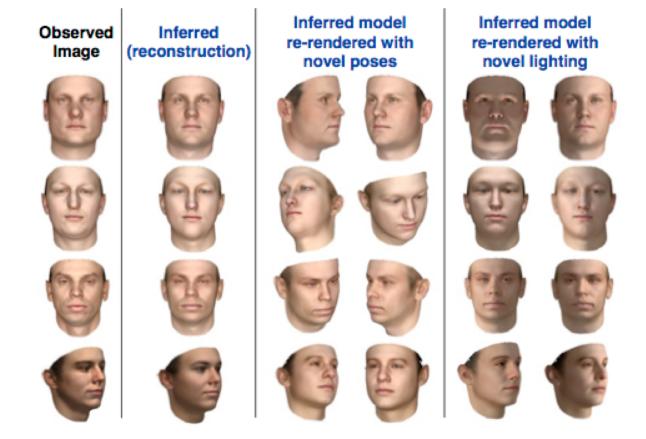
## Probabilistic programming with programmable inference

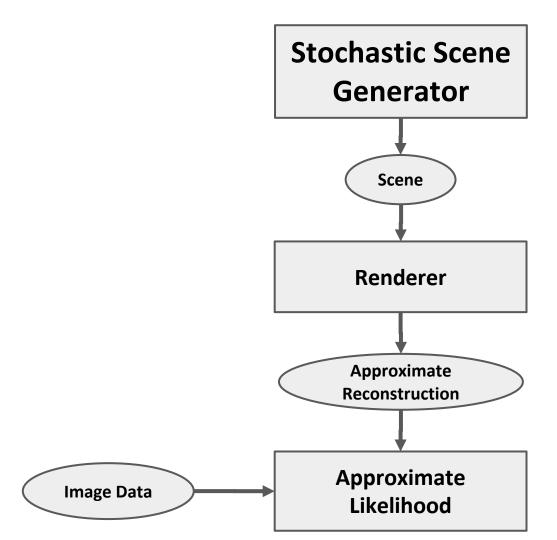


## Application: machine perception as inverse graphics

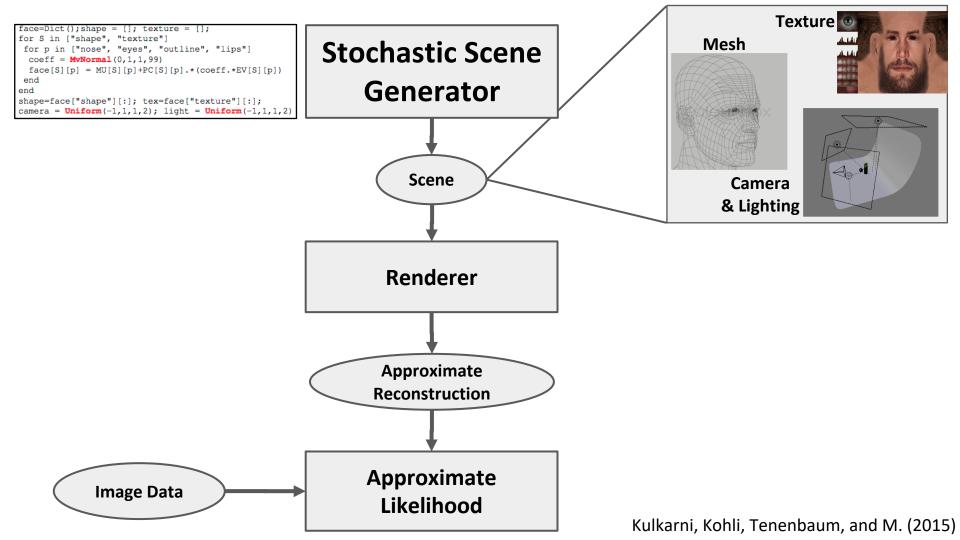


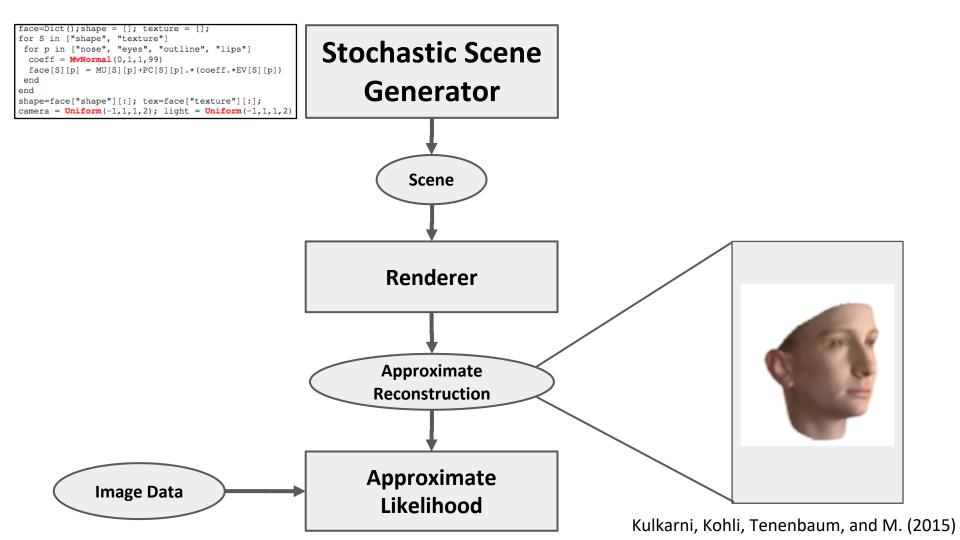
#### "What does this face look like from the side? Or when lit differently?"

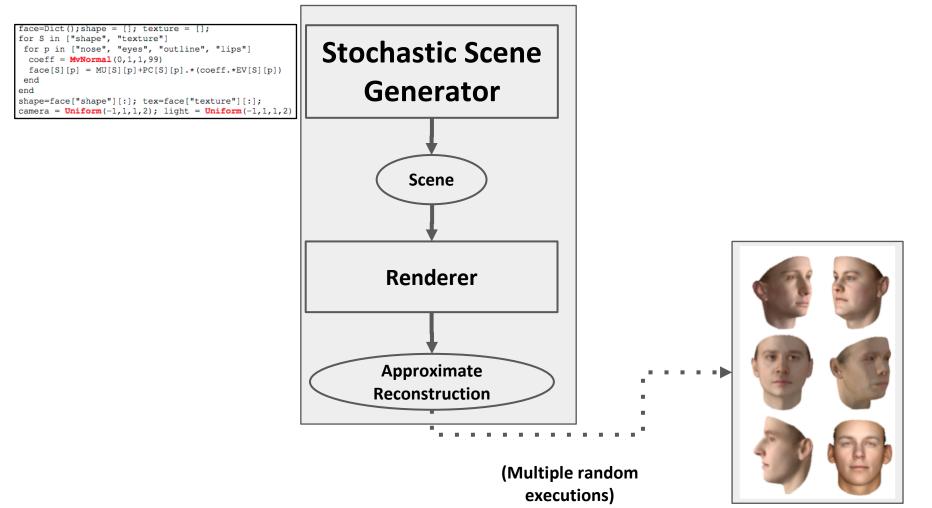




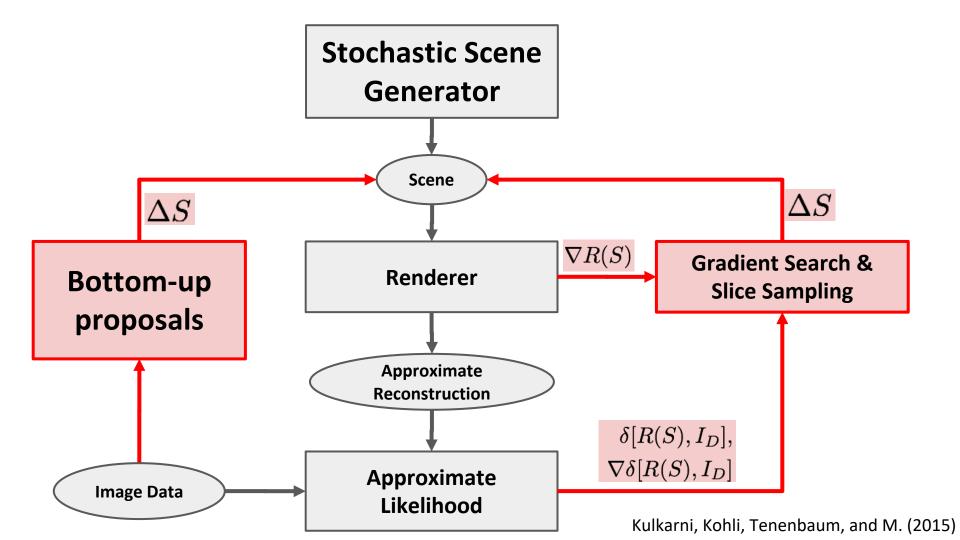
Kulkarni, Kohli, Tenenbaum, and M. (2015)

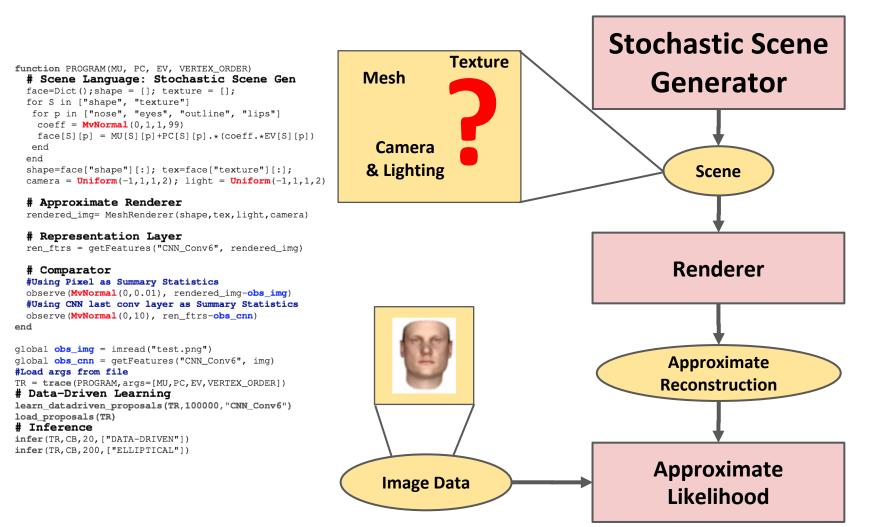




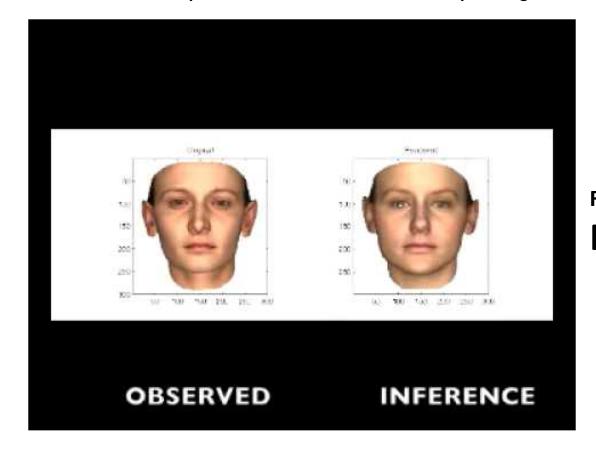


Kulkarni, Kohli, Tenenbaum, and M. (2015)





"Find a face shape and texture that matches this input image."



Input

Image

Reconstruction  $R(S) = I_R$ 

Kulkarni, Kohli, Tenenbaum, and Mansinghka (2015)

## Gen: a general-purpose probabilistic programming platform with programmable inference

#### Modeling and inference from multiple paradigms

Bayesian networks, Markov random fields, graphics/physics engines, deep neural network models

Monte Carlo inference, deep inference networks, numerical optimization

#### Programmable inference, not black-box

"Use Gibbs sampling to update X|Y, then optimize Y|X"

Advanced techniques, e.g. reversible jump and particle MCMC

Custom MCMC/SMC proposals, without requiring users to derive proposal densities and

#### Jacobians

Easy to combine built-in algorithms with arbitrary user-specified inference code

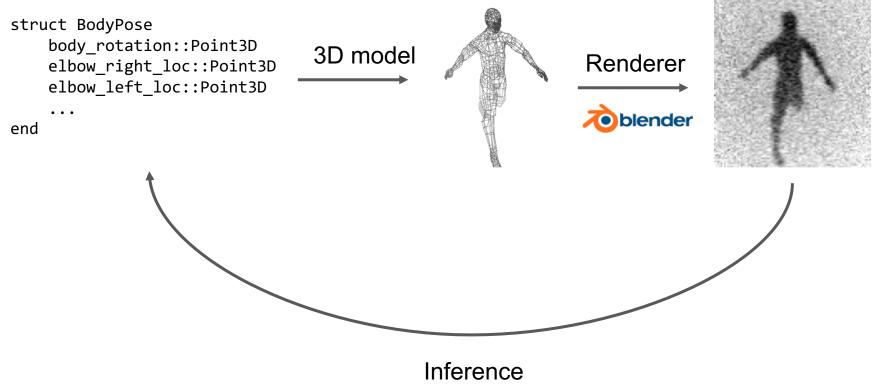
#### Fast enough for real-time applications

Out-of-the-box performance competitive with handwritten samplers

Users can optimize performance for slow components

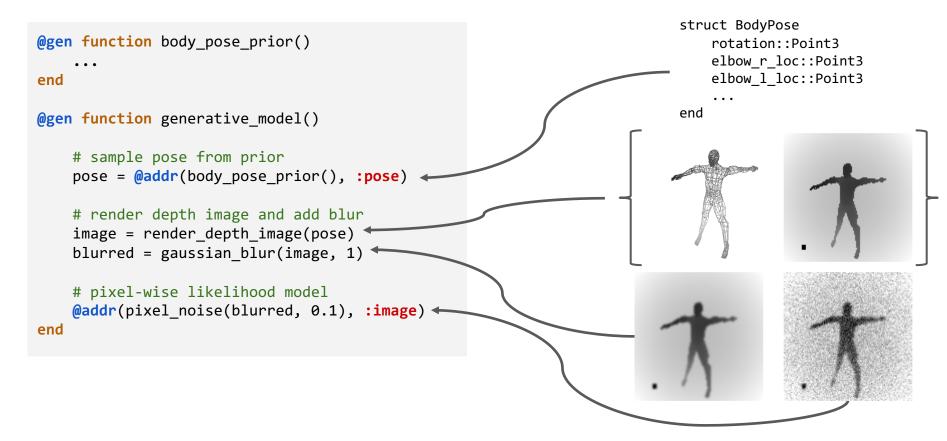
Cusumano-Towner et al. (2018)

## **Example: body pose inference as inverse graphics**



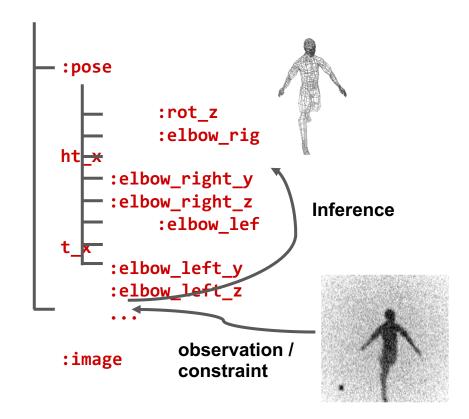
Cusumano-Towner et al. (2018)

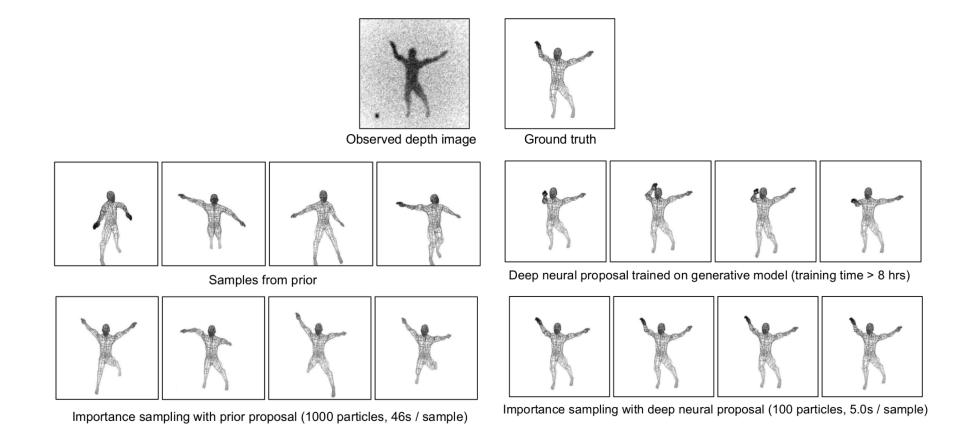
## Generative model based on a graphics engine



## Generative model based on a graphics engine

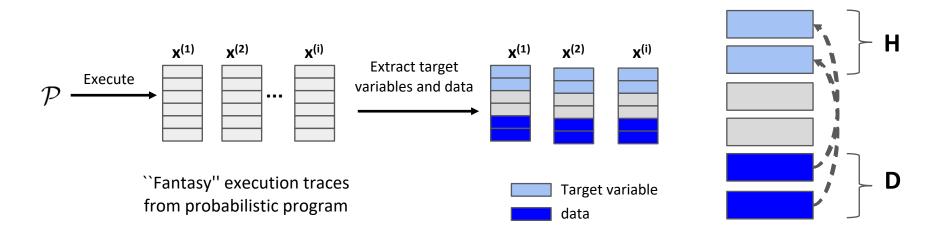
```
@gen function body pose prior()
end
@gen function generative model()
    # sample pose from prior
    pose = @addr(body pose prior(), :pose)
    # render depth image and add blur
    image = render depth image(pose)
    blurred = gaussian blur(image, 1)
    # pixel-wise likelihood model
    @addr(pixel noise(blurred, 0.1), :image)
end
```



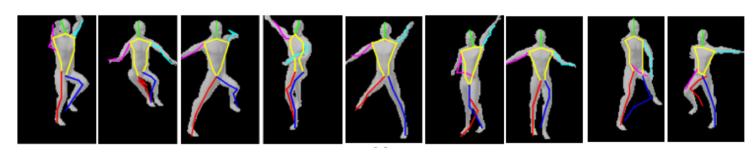


Cusumano-Towner et al. (2018)

## Inference using deep learning and Monte Carlo



#### Examples of ``fantasy" execution traces including target variables and data



## Challenge: integrating multiple modeling & inference paradigms

#### Monte Carlo in generative models

- Models defined by arbitrary generative code in Julia
- Fast editing of execution traces during MCMC inference, via incremental computation
- Fast resampling of execution traces for SMC inference, via persistent data structures

#### Deep learning

- Models defined by differentiable TensorFlow computations mixed with Julia code
- Batched gradients with respect to large parameter arrays located on GPU

#### **Gradient-based inference**

- Gradients with respect to ~10s of random variables (non-contiguous in memory)
- MAP, HMC, MALA, etc.

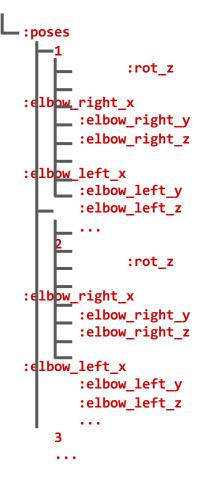
Cusumano-Towner et al. (2018)

```
@gen function neural_proposal_batched(images::Vector{Matrix{Float64}})

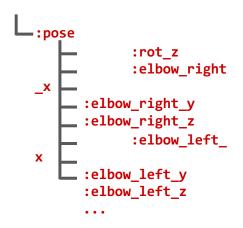
images_flat = vectorize_images(images)

# run inference network in batch
output_layer = @addr(neural_network(images_flat), :network)

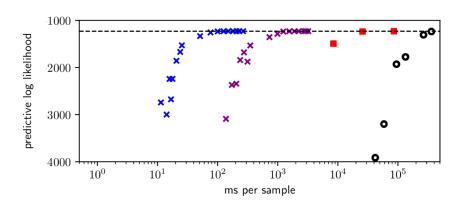
# make prediction for each image given inference network outputs
batch_size = length(images)
for i=1:batch_size
     @addr(predict_body_pose(outputs[i,:]), :poses => i)
end
end
```



```
@gen function neural proposal(image::Matrix{Float64})
    image flat = reshape(image, 1, 128 * 128)
    output layer = @addr(neural_network(image flat), :network)
    @addr(predict body pose(output layer[1,:]), :pose)
end
neural network = @tensorflow module begin
  @input image flat Float32 [-1, 128 * 128]
  image = tf.reshape(image flat, [-1, 128, 128, 1])
  @param W conv1 initial weight([5, 5, 1, 32])
  @param b conv1 initial bias([32])
  h conv1 = tf.nn.relu(conv2d(image, W conv1) + b conv1)
  h pool1 = max pool 2x2(h conv1)
  @param W fc1 initial weight([16 * 16 * 64, 1024])
  @param b fc1 initial bias([1024])
  h fc1 = tf.nn.relu(h pool3 flat * W fc1 + b fc1)
  @param W fc2 initial weight([1024, 32])
  @param b fc2 initial bias([32])
  @output Float32 (tf.matmul(h fc1, W fc2) + b fc2)
end
```

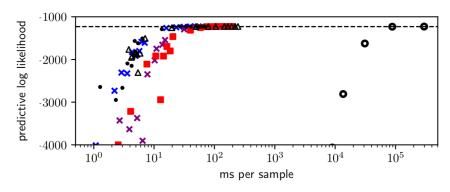


## Performance of Gen's JIT compiler



Gen-Static (MH+Gibbs)
 Gen-JIT (MH+Gibbs)
 Gen-Lite (MH+Gibbs)

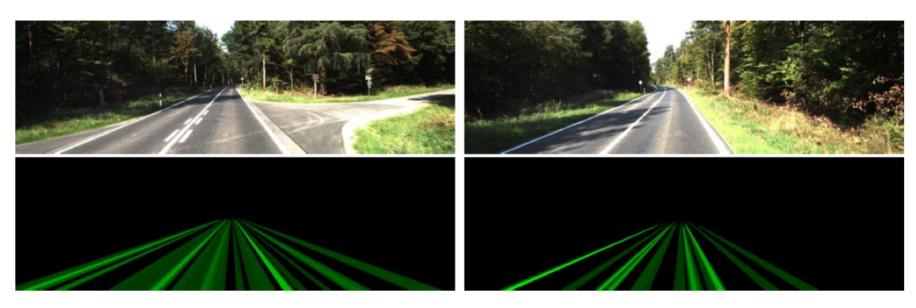
Uncollapsed model



★ Gen-Static (MH, collapsed)
 ★ Gen-JIT (MH, collapsed)
 ◆ Gen-Lite (MH, collapsed)
 ◆ Venture (MH, collapsed)

Manually collapsed model

Cusumano-Towner et al. (2018)



High uncertainty due to violated assumptions

Lower uncertainty for unsurprising data

## **Outline**

- 1. Motivation
- 2. What is probabilistic programming?

Pedagogical example: simple (or not-so-simple) curve fitting

3. Programmable inference, not just black-box

Application: machine perception via inverse graphics



4. Learning the structure and parameters of probabilistic programs

Application: automatic data modeling for scientific data analysis

5. The MIT Modeling and Inference Stack

#### Lab experiment



#### Experimental data

strain_name	time_point	temperature	Actuator_YFP	RiboJ00_Part_ribozyme	ybiT	ttdR	metR	cysM	preA
MG1655_Genomic_IcaR_Gate	18.0	37.0	7182.814030	23196.715220	56.407155	8.122473	3.404433	22.554367	13.138466
MG1655_Genomic_IcaR_Gate	18.0	37.0	6850.282154	20212.067980	66.983175	1.890360	4.621870	35.776926	7.134732
MG1655_Genomic_IcaR_Gate	18.0	37.0	6459.667717	12657.394760	105.104475	5.078912	6.622817	56.288495	14.057411
MG1655_Genomic_IcaR_Gate	18.0	37.0	5384.380877	10816.005350	78.503822	4.467902	6.991284	35.652097	14.164986
MG1655_Genomic_NAND_Circuit	18.0	37.0	29984.205560	57512.309870	83.724520	15.151475	43.165337	55.936072	14.918031
MG1655_Genomic_NAND_Circuit	18.0	37.0	34582.809280	87128.520830	101.577667	8.759255	20.559459	48.389122	13.223924
MG1655_Genomic_NAND_Circuit	18.0	37.0	31519.319620	76236.806450	126.530937	7.274019	23.475866	65.485309	17.021557
MG1655_Genomic_NAND_Circuit	18.0	37.0	35594.041500	114552.584000	90.227517	4.644846	29.526906	53.853729	8.181092
MG1655_Genomic_pTACmin	18.0	37.0	1616.725667	3313.110829	66.335180	7.078774	11.249797	29.872311	15.362400
MG1655_Genomic_pTACmin	18.0	37.0	1913.662092	4027.111166	82.239438	9.683810	15.389797	49.533963	11.878533

### Use cases for probabilistic programs that model a virtual experiment

- 1. Screen new batches of data for ETL errors and lab protocol execution errors
- 2. Detect drift between old and new batches of data
- 3. Detect multivariate relationships among experimental variables, and quantify their probable strength
- 4. Estimate anticipated variability in outcome for a given experimental condition

#### Hard to write

#### Experimental data

strain_name	time_point	temperature	Actuator_YFP	RiboJ00_Part_ribozyme	ybiT	ttdR	metR	cysM	preA
MG1655_Genomic_lcaR_Gate	18.0	37.0	7182.814030	23196.715220	56.407155	8.122473	3.404433	22.554367	13.138466
MG1655_Genomic_IcaR_Gate	18.0	37.0	6850.282154	20212.067980	66.983175	1.890360	4.621870	35.776926	7.134732
MG1655_Genomic_IcaR_Gate	18.0	37.0	6459.667717	12657.394760	105.104475	5.078912	6.622817	56.288495	14.057411
MG1655_Genomic_lcaR_Gate	18.0	37.0	5384.380877	10816.005350	78.503822	4.467902	6.991284	35.652097	14.164986
MG1655_Genomic_NAND_Circuit	18.0	37.0	29984.205560	57512.309870	83.724520	15.151475	43.165337	55.936072	14.918031
MG1655_Genomic_NAND_Circuit	18.0	37.0	34582.809280	87128.520830	101.577667	8.759255	20.559459	48.389122	13.223924
MG1655_Genomic_NAND_Circuit	18.0	37.0	31519.319620	76236.806450	126.530937	7.274019	23.475866	65.485309	17.021557
MG1655_Genomic_NAND_Circuit	18.0	37.0	35594.041500	114552.584000	90.227517	4.644846	29.526906	53.853729	8.181092
MG1655_Genomic_pTACmin	18.0	37.0	1616.725667	3313.110829	66.335180	7.078774	11.249797	29.872311	15.362400
MG1655_Genomic_pTACmin	18.0	37.0	1913.662092	4027.111166	82.239438	9.683810	15.389797	49.533963	11.87853



#### Experimental data

strain_name	time_point	temperature	Actuator_YFP	RiboJ00_Part_ribozyme	ybiT	ttdR	metR	cysM	preA
MG1655_Genomic_IcaR_Gate	18.0	37.0	7182.814030	23196.715220	56.407155	8.122473	3.404433	22.554367	13.138466
MG1655_Genomic_IcaR_Gate	18.0	37.0	6850.282154	20212.067980	66.983175	1.890360	4.621870	35.776926	7.134732
MG1655_Genomic_IcaR_Gate	18.0	37.0	6459.667717	12657.394760	105.104475	5.078912	6.622817	56.288495	14.057411
MG1655_Genomic_IcaR_Gate	18.0	37.0	5384.380877	10816.005350	78.503822	4.467902	6.991284	35.652097	14.164986
MG1655_Genomic_NAND_Circuit	18.0	37.0	29984.205560	57512.309870	83.724520	15.151475	43.165337	55.936072	14.918031
MG1655_Genomic_NAND_Circuit	18.0	37.0	34582.809280	87128.520830	101.577667	8.759255	20.559459	48.389122	13.223924
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MG1655_Genomic_pTACmin	18.0	37.0	1616.725667	3313.110829	66.335180	7.078774	11.249797	29.872311	15.362400
MG1655_Genomic_pTACmin	18.0	37.0	1913.662092	4027.111166	82.239438	9.683810	15.389797	49.533963	11.878533

```
(define generate-virtual-experimental-results-using-model-1
  (gen []

  (define cluster-for-actuator_yfp-and-riboj00_part_ribozyme (
        categorical [0.62 0.29 0.09]))

  (define [actuator_yfp-mean actuator_yfp-std] (cond
        (= cluster-for-actuator_yfp-and-riboj00_part_ribozyme 0) [34278.55 63904.74]
        (= cluster-for-actuator_yfp-and-riboj00_part_ribozyme 1) [0.0 0.01]
        (= cluster-for-actuator_yfp-and-riboj00_part_ribozyme 2) [336058.53125 432304.475202]))
        (define actuator_yfp (gaussian actuator_yfp-mean actuator_yfp-std))

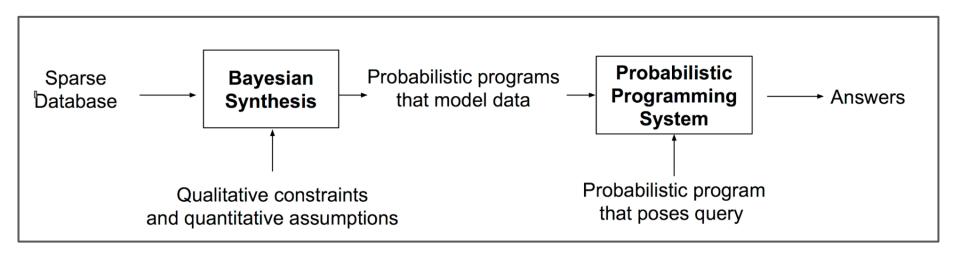
        (define [riboi00 part ribozyme-mean riboi00 part ribozyme-std] (cond)
```

# Can we automatically build probabilistic programs that model the data?

#### Experimental data

strain_name	time_point	temperature	Actuator_YFP	RiboJ00_Part_ribozyme	ybiT	ttdR	metR	cysM	preA
MG1655_Genomic_lcaR_Gate	18.0	37.0	7182.814030	23196.715220	56.407155	8.122473	3.404433	22.554367	13.138466
MG1655_Genomic_lcaR_Gate	18.0	37.0	6850.282154	20212.067980	66.983175	1.890360	4.621870	35.776926	7.134732
MG1655_Genomic_lcaR_Gate	18.0	37.0	6459.667717	12657.394760	105.104475	5.078912	6.622817	56.288495	14.057411
MG1655_Genomic_lcaR_Gate	18.0	37.0	5384.380877	10816.005350	78.503822	4.467902	6.991284	35.652097	14.164986
MG1655_Genomic_NAND_Circuit	18.0	37.0	29984.205560	57512.309870	83.724520	15.151475	43.165337	55.936072	14.918031
MG1655_Genomic_NAND_Circuit	18.0	37.0	34582.809280	87128.520830	101.577667	8.759255	20.559459	48.389122	13.223924
MG1655_Genomic_NAND_Circuit	18.0	37.0	31519.319620	76236.806450	126.530937	7.274019	23.475866	65.485309	17.021557
MG1655_Genomic_NAND_Circuit	18.0	37.0	35594.041500	114552.584000	90.227517	4.644846	29.526906	53.853729	8.181092
MG1655_Genomic_pTAC	100	^-^	16.725667	3313.110829	66.335180	7.078774	11.249797	29.872311	15.362400
MG1655_Genomic_pTA0			13.662092	4027.111166	82.239438	9.683810	15.389797	49.533963	11.878533

# Automated data modeling for science via Bayesian probabilistic program synthesis



Mansinghka et al. (arXiv 2015)
Mansinghka et al. (JMLR 2016)
Saad & Mansinghka (NIPS 2016)
Saad & Mansinghka (AISTATS 2017)
Saad & Schaechtle et al. (under review; arXiv 2017)

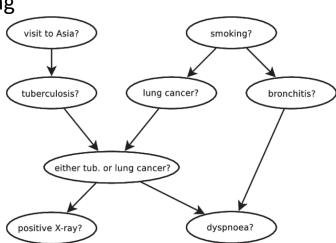


## Technical challenge: structure learning is hard...

Robust automatic data modeling requires learning model structure, not just parameters...

Remember Bayesian network structure learning:

- Search over structures was slow and unreliable
- Hard to include hidden variables, leading to underfitting
- Hard to apply to mixed numerical and discrete data
- Hard to get uncertainty over model structure



## ... but we can use tools from nonparametric Bayes!

10 years of research & engineering towards CrossCat, a nonparametric Bayesian prior over probabilistic model structure and parameters.

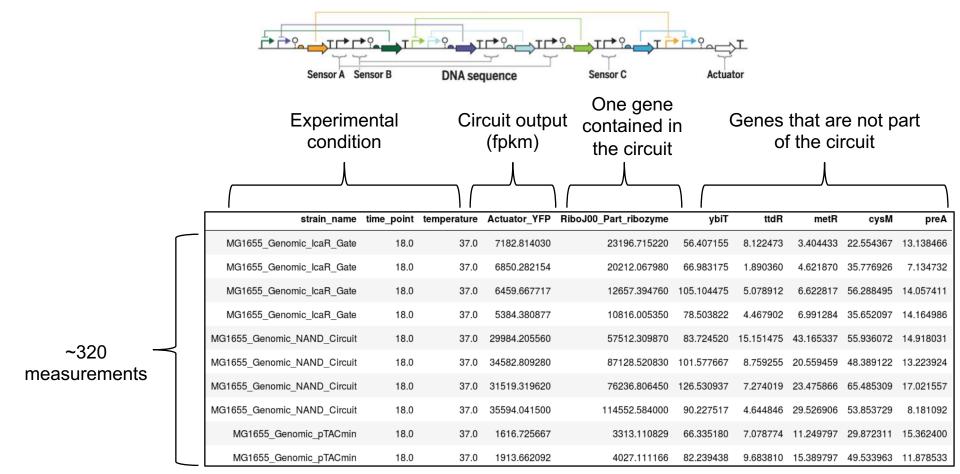
Monte Carlo implementation scales to tables with ~100K rows and ~1K columns

$$\begin{split} \alpha_D \sim \operatorname{Gamma}(k=1,\theta=1) \\ \vec{\lambda}_d \sim \ V_d(\cdot) & \text{for each } d \in \{1,\cdots,D\} \\ z_d \sim \ \operatorname{CRP}(\{z_i \mid i \neq d\}; \alpha_D) & \text{for each } d \in \{1,\cdots,D\} \\ \alpha_v \sim \ \operatorname{Gamma}(k=1,\theta=1) & \text{for each } v \in \vec{z} \\ y_r^v \sim \ \operatorname{CRP}(\{y_i^v \mid i \neq r\}; \alpha_v) & \text{for each } v \in \vec{z} \text{ and } \\ r \in \{1,\cdots,R\} \\ \vec{\theta_c}^d \sim \ M_d(\cdot; \vec{\lambda}_d) & \text{for each } v \in \vec{z}, c \in \vec{y}^v, \text{ and } d \text{ such that } \\ z_d = v \text{ and } u_d = 1 \\ \vec{x}_{(\cdot,d)}^c = \{x_{(r,d)} \mid y_r^{z_d} = c\} \sim \begin{cases} \prod_r L_d(\vec{\theta_c}^d) & \text{if } u_d = 1 \\ ML_d(\vec{\lambda}_d) & \text{if } u_d = 0 \end{cases} & \text{for each } v \in \vec{z} \text{ and each } c \in \vec{y}^v \end{split}$$

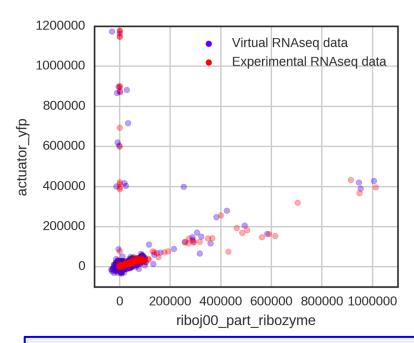
Mansinghka et al. (JMLR 2016; NIPS 2009; CogSci 2006);

Obermeyer et al. (AISTATS; 2014);

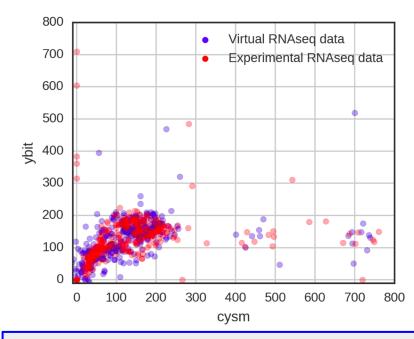
## Example dataset from genetic circuit design



## Compare virtual and experimental RNAseq data



%%bql
SELECT riboj00\_part\_ribozyme, actuator\_yfp
 FROM data;



%%bql
SIMULATE cysm, ybit FROM data;

%%bql
SELECT cysm, ybit FROM data;

In less than 20 lines of code, we generate probabilistic programs to model a new dataset.

```
%%bq1
CREATE TABLE "data subset" AS
    SELECT
        "Actuator_yfp",
        "riboj00 part ribozyme",
        "Ybit",
        "cysM" FROM "data"
CREATE POPULATION FOR "data subset" WITH SCHEMA (
     SET STATTYPES OF
          "Actuator YFP",
          "riboj00 part ribozyme",
          "ybiT",
          "cysM" TO NUMERICAL);
CREATE GENERATOR FOR "data subset";
INITIALIZE 100 MODELS;
ANALYZE "data subset" FOR 50 ITERATIONS;
%%python
```

code = export to metaprob("data subset")

For this demo, we use a subset of all the data available, namely:

- 1. A part of the circuit and YFP; and
- 2. Two genes that weren't part of the circuit and should not have interactions with it YFP.

```
%%bql
CREATE TABLE "data_subset" AS
    SELECT
        "Actuator_yfp",
        "riboj00_part_ribozyme",
        "Ybit",
        "cysM" FROM "data"
```

```
CREATE POPULATION FOR "data subset" WITH SCHEMA (
     SET STATTYPES OF
          "Actuator YFP",
          "riboj00 part ribozyme",
          "vbiT",
          "cysM" TO NUMERICAL);
CREATE GENERATOR FOR "data subset";
INITIALIZE 100 MODELS;
ANALYZE "data subset" FOR 50 ITERATIONS;
%%python
code = export to metaprob("data subset")
```

We create a statistical population for this data

```
CREATE POPULATION FOR "data_subset" WITH SCHEMA (
    SET STATTYPES OF
        "Actuator_YFP",
        "riboj00_part_ribozyme",
        "ybiT",
        "cysM" TO NUMERICAL);
```

```
CREATE GENERATOR FOR "data_subset";
INITIALIZE 100 MODELS;
ANALYZE "data_subset" FOR 50 ITERATIONS;

%%python
code = export_to_metaprob("data_subset")
```

```
%%bql
CREATE TABLE "data subset" AS
    SELECT
        "Actuator_yfp",
        "riboj00 part ribozyme",
        "Ybit",
        "cysM" FROM "data"
CREATE POPULATION FOR "data subset" WITH SCHEMA (
     SET STATTYPES OF
          "Actuator YFP",
          "riboj00 part ribozyme",
          "ybiT",
          "cysM" TO NUMERICAL);
```

```
Run analysis on an ensemble of 100 models
```

```
CREATE GENERATOR FOR "data_subset";
INITIALIZE 100 MODELS;
ANALYZE "data_subset" FOR 50 ITERATIONS;
```

```
%%python
code = export_to_metaprob("data_subset")
```

```
%%bql
CREATE TABLE "data subset" AS
    SELECT
        "Actuator_yfp",
        "riboj00 part ribozyme",
        "Ybit",
        "cysM" FROM "data"
CREATE POPULATION FOR "data subset" WITH SCHEMA (
     SET STATTYPES OF
          "Actuator YFP",
          "riboj00 part ribozyme",
          "ybiT",
          "cysM" TO NUMERICAL);
CREATE GENERATOR FOR "data subset";
INITIALIZE 100 MODELS;
ANALYZE "data subset" FOR 50 ITERATIONS;
```

Export the learned ensemble of models to Metaprob

%%python
code = export\_to\_metaprob("data\_subset")

```
(define cluster-for-actuator yfp-and-riboj00 part ribozyme (
                                                             categorical [0.62 0.29 0.09]))
                                                         (define [actuator yfp-mean actuator yfp-std] (cond
                                                           (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [34278.55 63904.74]
                                                           (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
                                                           (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [336058.53125 432304.475202]))
                                                         (define actuator yfp (gaussian actuator yfp-mean actuator yfp-std))
                                                         (define [riboj00 part ribozyme-mean riboj00 part ribozyme-std] (cond
                                                           (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [83284.60 63904.74]
                                                           (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
                                                           (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [0.0 0.01]))
                                                         (define riboj00 part ribozyme
                                                             (gaussian riboj00 part ribozyme-mean riboj00 part ribozyme-std))
The result of synthesis:
                                                         (define cluster-for-ybit-and-cysm (categorical [0.59 0.24 0.09 0.05 0.02 0.01]))
       executable with Metaprob;
                                                         (define [ybit-mean ybit-std] (cond
       human readable; and
                                                           (= cluster-for-ybit-and-cysm 0) [149.01 46.92]
       editable.
                                                           (= cluster-for-ybit-and-cysm 1) [72.21 15.56]
                                                           (= cluster-for-ybit-and-cysm 2) [185.27 302.73]
                                                           (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
                                                           (= cluster-for-ybit-and-cysm 4) [762.128173828 0.01]
                                                           (= cluster-for-ybit-and-cysm 5) [0.0 0.01]))
                                                         (define vbit (gaussian vbit-mean vbit-std))
                                                         (define [cvsm-mean cvsm-std] (cond
                                                           (= cluster-for-ybit-and-cysm 0) [150.76 46.92]
                                                           (= cluster-for-ybit-and-cysm 1) [43.56 15.56]
                                                           (= cluster-for-ybit-and-cysm 2) [641.10 302.73]
                                                           (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
                                                           (= cluster-for-ybit-and-cysm 4) [0.0 0.01]
                                                           (= cluster-for-ybit-and-cysm 5) [813.07 420.35]))
                                                         (define cysm (gaussian cysm-mean cysm-std))
```

virtual-experimental-results))

(gen []

define generate-virtual-experimental-results-using-model-1

(define virtual-experimental-results [actuator yfp riboj00 part ribozyme ybit cysm])

The bql code above learned an ensemble of 100 models. We inspect the code for one of them (model #1).

```
(define generate-virtual-experimental-results-using-model-1
 (gen []
   (define cluster-for-actuator yfp-and-riboj00 part ribozyme (
       categorical [0.62 0.29 0.09]))
   (define [actuator yfp-mean actuator yfp-std] (cond
     (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [34278.55 63904.74]
     (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
     (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [336058.53125 432304.475202]))
   (define actuator yfp (gaussian actuator yfp-mean actuator yfp-std))
   (define [riboj00 part ribozyme-mean riboj00 part ribozyme-std] (cond
     (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [83284.60 63904.74]
     (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
     (= cluster-for-actuator vfp-and-riboi00 part ribozyme 2) [0.0 0.01]))
   (define riboj00 part ribozyme
       (gaussian riboj00 part ribozyme-mean riboj00 part ribozyme-std))
   (define cluster-for-ybit-and-cysm (categorical [0.59 0.24 0.09 0.05 0.02 0.01]))
   (define [ybit-mean ybit-std] (cond)
     (= cluster-for-ybit-and-cysm 0) [149.01 46.92]
     (= cluster-for-ybit-and-cysm 1) [72.21 15.56]
     (= cluster-for-ybit-and-cysm 2) [185.27 302.73]
     (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
     (= cluster-for-ybit-and-cysm 4) [762.128173828 0.01]
     (= cluster-for-ybit-and-cysm 5) [0.0 0.01]))
   (define vbit (gaussian vbit-mean vbit-std))
   (define [cysm-mean cysm-std] (cond)
     (= cluster-for-ybit-and-cysm 0) [150.76 46.92]
     (= cluster-for-ybit-and-cysm 1) [43.56 15.56]
     (= cluster-for-ybit-and-cysm 2) [641.10 302.73]
     (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
     (= cluster-for-ybit-and-cysm 4) [0.0 0.01]
     (= cluster-for-ybit-and-cysm 5) [813.07 420.35]))
   (define cysm (gaussian cysm-mean cysm-std))
   (define virtual-experimental-results [actuator vfp riboj00 part ribozyme vbit cysm])
   virtual-experimental-results))
```

The learned model indicates that actuator\_yfp and riboj00\_part\_ribozyme are dependent variables.

This implies that for those two variables, we synthesized a 2-d Gaussian mixture model.

To sample new values for actuator\_yfp and riboj00\_part\_ribozyme, we first need to sample the mixture component (cluster).

```
(define generate-virtual-experimental-results-using-model-1
  (gen []
    (define cluster-for-actuator yfp-and-riboj00 part ribozyme (
        categorical [0.62 0.29 0.09]))
    (define [actuator yfp-mean actuator yfp-std] (cond
      (= cluster-for-actuator_yfp-and-riboj00_part_ribozyme 0) [34278.55 63904.74]
     (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [336058.53125 432304.475202]))
    (define actuator yfp (gaussian actuator yfp-mean actuator yfp-std))
    (define [riboj00 part ribozyme-mean riboj00 part ribozyme-std] (cond
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [83284.60 63904.74]
     (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [0.0 0.01]))
    (define riboj00 part ribozyme
        (gaussian riboj00 part ribozyme-mean riboj00 part ribozyme-std))
    (define cluster-for-ybit-and-cysm (categorical [0.59 0.24 0.09 0.05 0.02 0.01]))
    (define [ybit-mean ybit-std] (cond)
      (= cluster-for-ybit-and-cysm 0) [149.01 46.92]
      (= cluster-for-ybit-and-cysm 1) [72.21 15.56]
      (= cluster-for-ybit-and-cysm 2) [185.27 302.73]
      (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 4) [762.128173828 0.01]
      (= cluster-for-ybit-and-cysm 5) [0.0 0.01]))
    (define vbit (gaussian vbit-mean vbit-std))
    (define [cysm-mean cysm-std] (cond)
      (= cluster-for-ybit-and-cysm 0) [150.76 46.92]
      (= cluster-for-ybit-and-cysm 1) [43.56 15.56]
      (= cluster-for-ybit-and-cysm 2) [641.10 302.73]
      (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 4) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 5) [813.07 420.35]))
    (define cysm (gaussian cysm-mean cysm-std))
    (define virtual-experimental-results [actuator vfp riboj00 part ribozyme vbit cysm])
    virtual-experimental-results)
```

The parametrization, i.e. mean and standard deviation (std) of the Gaussian components for the mixture model for actuator\_yfp depends on the previously sampled cluster id, (cluster-for-actuator\_yfp -and-ribojo00-part\_ribyzmye).

```
(define generate-virtual-experimental-results-using-model-1
  (gen []
    (define cluster-for-actuator yfp-and-riboj00 part ribozyme (
        categorical [0.62 0.29 0.09]))
    (define [actuator yfp-mean actuator yfp-std] (cond
      (= cluster-for-actuator_yfp-and-riboj00_part_ribozyme 0) [34278.55 63904.74]
      (= cluster-for-actuator_yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [336058.53125 432304.475202]))
    (define actuator yfp (gaussian actuator yfp-mean actuator yfp-std))
    (define [riboj00 part ribozyme-mean riboj00 part ribozyme-std] (cond
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [83284.60 63904.74]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator vfp-and-riboj00 part ribozyme 2) [0.0 0.01]))
    (define riboj00 part ribozyme
        (gaussian riboj00 part ribozyme-mean riboj00 part ribozyme-std))
    (define cluster-for-ybit-and-cysm (categorical [0.59 0.24 0.09 0.05 0.02 0.01]))
    (define [ybit-mean ybit-std] (cond)
      (= cluster-for-ybit-and-cysm 0) [149.01 46.92]
      (= cluster-for-ybit-and-cysm 1) [72.21 15.56]
      (= cluster-for-ybit-and-cysm 2) [185.27 302.73]
      (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 4) [762.128173828 0.01]
      (= cluster-for-ybit-and-cysm 5) [0.0 0.01]))
    (define vbit (gaussian vbit-mean vbit-std))
    (define [cysm-mean cysm-std] (cond)
      (= cluster-for-ybit-and-cysm 0) [150.76 46.92]
      (= cluster-for-ybit-and-cysm 1) [43.56 15.56]
      (= cluster-for-ybit-and-cysm 2) [641.10 302.73]
      (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 4) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 5) [813.07 420.35]))
    (define cysm (gaussian cysm-mean cysm-std))
    (define virtual-experimental-results [actuator vfp riboj00 part ribozyme vbit cysm])
    virtual-experimental-results)
```

We now sample a value for actuator\_yfp from a Gaussian with the previously determined mean and standard deviation.

```
(define generate-virtual-experimental-results-using-model-1
  (gen []
    (define cluster-for-actuator yfp-and-riboj00 part ribozyme (
        categorical [0.62 0.29 0.09]))
    (define [actuator yfp-mean actuator yfp-std] (cond
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [34278.55 63904.74]
     (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [336058.53125 432304.475202]))
    (define actuator yfp (gaussian actuator yfp-mean actuator yfp-std))
    (define [riboj00 part ribozyme-mean riboj00 part ribozyme-std] (cond
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [83284.60 63904.74]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator vfp-and-riboj00 part ribozyme 2) [0.0 0.01]))
    (define riboj00 part ribozyme
        (gaussian riboj00 part ribozyme-mean riboj00 part ribozyme-std))
    (define cluster-for-ybit-and-cysm (categorical [0.59 0.24 0.09 0.05 0.02 0.01]))
    (define [ybit-mean ybit-std] (cond)
      (= cluster-for-ybit-and-cysm 0) [149.01 46.92]
      (= cluster-for-ybit-and-cysm 1) [72.21 15.56]
      (= cluster-for-ybit-and-cysm 2) [185.27 302.73]
      (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 4) [762.128173828 0.01]
      (= cluster-for-ybit-and-cysm 5) [0.0 0.01]))
    (define vbit (gaussian vbit-mean vbit-std))
    (define [cysm-mean cysm-std] (cond)
      (= cluster-for-ybit-and-cysm 0) [150.76 46.92]
     (= cluster-for-ybit-and-cysm 1) [43.56 15.56]
      (= cluster-for-ybit-and-cysm 2) [641.10 302.73]
      (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
     (= cluster-for-ybit-and-cysm 4) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 5) [813.07 420.35]))
    (define cysm (gaussian cysm-mean cysm-std))
    (define virtual-experimental-results [actuator vfp riboj00 part ribozyme vbit cysm])
    virtual-experimental-results))
```

riboj00\_part \_ribozyme and actuator\_yfp are dependent. We use the same cluster id we sampled previously to determine mean and standard deviation for the gaussian component.

We then sample a value for riboj00\_part \_ribozyme from an accordingly parameterized Gaussian component.

```
(define generate-virtual-experimental-results-using-model-1
  (gen []
    (define cluster-for-actuator yfp-and-riboj00 part ribozyme (
        categorical [0.62 0.29 0.09]))
    (define [actuator yfp-mean actuator yfp-std] (cond
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [34278.55 63904.74]
     (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [336058.53125 432304.475202]))
    (define actuator yfp (gaussian actuator yfp-mean actuator yfp-std))
    (define [riboj00 part_ribozyme-mean riboj00_part_ribozyme-std] (cond)
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [83284.60 63904.74]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [0.0 0.01]))
    (define riboj00 part ribozyme
        (gaussian riboj00 part ribozyme-mean riboj00 part ribozyme-std))
    (define cluster-for-ybit-and-cysm (categorical [0.59 0.24 0.09 0.05 0.02 0.01]))
    (define [ybit-mean ybit-std] (cond)
      (= cluster-for-ybit-and-cysm 0) [149.01 46.92]
      (= cluster-for-ybit-and-cysm 1) [72.21 15.56]
      (= cluster-for-ybit-and-cysm 2) [185.27 302.73]
      (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 4) [762.128173828 0.01]
      (= cluster-for-ybit-and-cysm 5) [0.0 0.01]))
    (define vbit (gaussian vbit-mean vbit-std))
    (define [cysm-mean cysm-std] (cond)
      (= cluster-for-ybit-and-cysm 0) [150.76 46.92]
      (= cluster-for-ybit-and-cysm 1) [43.56 15.56]
      (= cluster-for-ybit-and-cysm 2) [641.10 302.73]
      (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 4) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 5) [813.07 420.35]))
    (define cysm (gaussian cysm-mean cysm-std))
    (define virtual-experimental-results [actuator yfp riboj00 part ribozyme ybit cysm])
    virtual-experimental-results))
```

The learned model indicates that ybit and cysm are dependent variables; but independent from actuator\_yfp and riboj00\_part\_ribozyme.

We sample a new, different cluster id for ybit and cysm.

```
(define generate-virtual-experimental-results-using-model-1
  (gen []
    (define cluster-for-actuator yfp-and-riboj00 part ribozyme (
        categorical [0.62 0.29 0.09]))
    (define [actuator yfp-mean actuator yfp-std] (cond
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [34278.55 63904.74]
     (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [336058.53125 432304.475202]))
    (define actuator yfp (gaussian actuator yfp-mean actuator yfp-std))
    (define [riboj00 part ribozyme-mean riboj00 part ribozyme-std] (cond
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [83284.60 63904.74]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [0.0 0.01]))
    (define riboj00 part ribozyme
        (gaussian riboj00 part ribozyme-mean riboj00 part ribozyme-std))
    (define cluster-for-ybit-and-cysm (categorical [0.59 0.24 0.09 0.05 0.02 0.01]))
    (define [ybit-mean ybit-std] (cond)
      (= cluster-for-ybit-and-cysm 0) [149.01 46.92]
      (= cluster-for-ybit-and-cysm 1) [72.21 15.56]
      (= cluster-for-ybit-and-cysm 2) [185.27 302.73]
      (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 4) [762.128173828 0.01]
      (= cluster-for-ybit-and-cysm 5) [0.0 0.01]))
    (define vbit (gaussian vbit-mean vbit-std))
    (define [cysm-mean cysm-std] (cond)
      (= cluster-for-ybit-and-cysm 0) [150.76 46.92]
      (= cluster-for-ybit-and-cysm 1) [43.56 15.56]
      (= cluster-for-ybit-and-cysm 2) [641.10 302.73]
      (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 4) [0.0 0.01]
      (= cluster-for-ybit-and-cysm 5) [813.07 420.35]))
    (define cysm (gaussian cysm-mean cysm-std))
    (define virtual-experimental-results [actuator vfp riboj00 part ribozyme vbit cysm])
    virtual-experimental-results))
```

```
(define generate-virtual-experimental-results-using-model-1
  (gen []
    (define cluster-for-actuator yfp-and-riboj00 part ribozyme (
        categorical [0.62 0.29 0.09]))
    (define [actuator yfp-mean actuator yfp-std] (cond
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [34278.55 63904.74]
     (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [336058.53125 432304.475202]))
    (define actuator yfp (gaussian actuator yfp-mean actuator yfp-std))
    (define [riboj00 part ribozyme-mean riboj00 part ribozyme-std] (cond
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [83284.60 63904.74]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
      (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [0.0 0.01]))
    (define riboj00 part ribozyme
        (gaussian riboj00 part ribozyme-mean riboj00 part ribozyme-std))
    (define cluster-for-ybit-and-cysm (categorical [0.59 0.24 0.09 0.05 0.02 0.01]))
    (define [ybit-mean ybit-std] (cond
```

(define virtual-experimental-results [actuator vfp riboj00 part ribozyme vbit cysm])

Repeat the process from above and draw values from one Gaussian for ybit and from another for cysm with parameters that depend on the value of cluster-for-ybit-and-cysm.

virtual-experimental-results))

```
(define cluster-for-actuator yfp-and-riboj00 part ribozyme (
                                                             categorical [0.62 0.29 0.09]))
                                                         (define [actuator yfp-mean actuator yfp-std] (cond
                                                           (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [34278.55 63904.74]
                                                           (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
                                                           (= cluster-for-actuator yfp-and-riboj00 part ribozyme 2) [336058.53125 432304.475202]))
                                                         (define actuator vfp (gaussian actuator vfp-mean actuator vfp-std))
                                                         (define [riboj00 part ribozyme-mean riboj00 part ribozyme-std] (cond
                                                           (= cluster-for-actuator yfp-and-riboj00 part ribozyme 0) [83284.60 63904.74]
                                                           (= cluster-for-actuator yfp-and-riboj00 part ribozyme 1) [0.0 0.01]
                                                           (= cluster-for-actuator vfp-and-riboj00 part ribozyme 2) [0.0 0.01]))
                                                         (define riboj00 part ribozyme
                                                             (gaussian riboj00 part ribozyme-mean riboj00 part ribozyme-std))
                                                         (define cluster-for-ybit-and-cysm (categorical [0.59 0.24 0.09 0.05 0.02 0.01]))
                                                         (define [ybit-mean ybit-std] (cond)
                                                           (= cluster-for-ybit-and-cysm 0) [149.01 46.92]
                                                           (= cluster-for-ybit-and-cysm 1) [72.21 15.56]
                                                           (= cluster-for-ybit-and-cysm 2) [185.27 302.73]
                                                           (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
                                                           (= cluster-for-ybit-and-cysm 4) [762.128173828 0.01]
                                                           (= cluster-for-ybit-and-cysm 5) [0.0 0.01]))
                                                         (define vbit (gaussian vbit-mean vbit-std))
                                                         (define [cvsm-mean cvsm-std] (cond
We return the virtual experiment results,
                                                           (= cluster-for-ybit-and-cysm 0) [150.76 46.92]
                                                           (= cluster-for-ybit-and-cysm 1) [43.56 15.56]
i.e. the sampled values for:
                                                           (= cluster-for-ybit-and-cysm 2) [641.10 302.73]
       actuator yfp
                                                           (= cluster-for-ybit-and-cysm 3) [0.0 0.01]
                                                           (= cluster-for-ybit-and-cysm 4) [0.0 0.01]
       riboj00 part ribozyme
                                                           (= cluster-for-ybit-and-cysm 5) [813.07 420.35]))
       ybit
                                                         (define cysm (gaussian cysm-mean cysm-std))
       cysm
                                                         (define virtual-experimental-results [actuator yfp riboj00 part ribozyme ybit cysm])
                                                         virtual-experimental-results))
```

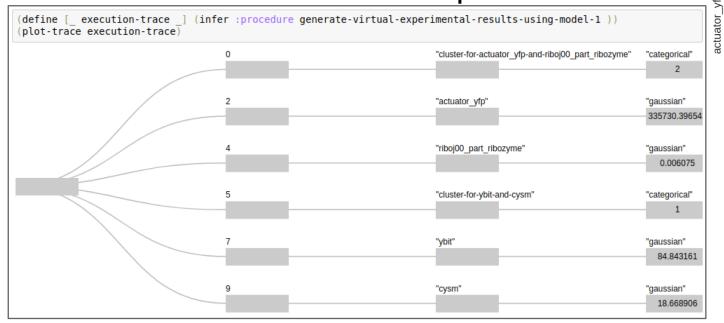
(gen []

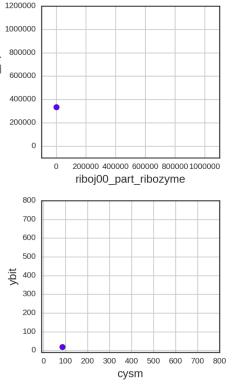
(define generate-virtual-experimental-results-using-model-1

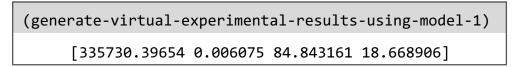
(generate-virtual-experimental-results-using-model-1)

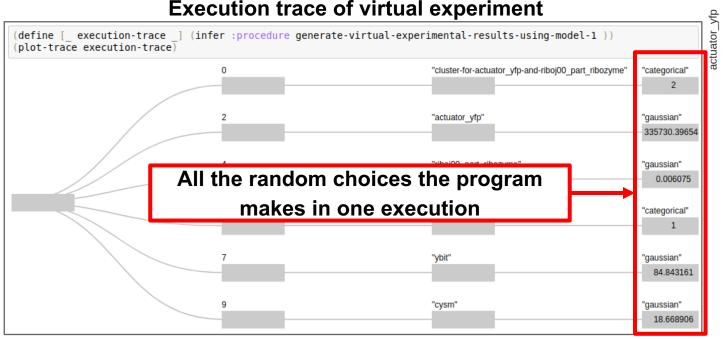
[335730.39654 0.006075 84.843161 18.668906]

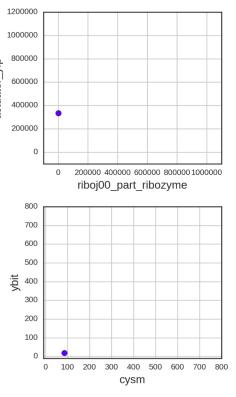
### **Execution trace of virtual experiment**





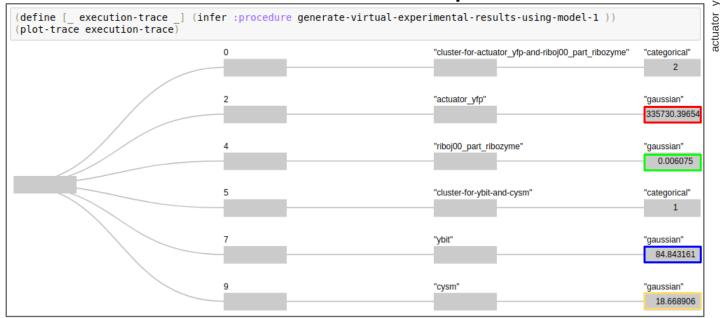


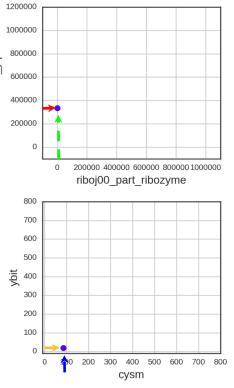




(generate-virtual-experimental-results-using-model-1)
[335730.39654 0.006075 84.843161 18.668906]

### **Execution trace of virtual experiment**



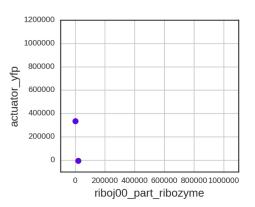


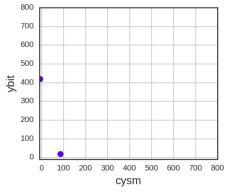
(generate-virtual-experimental-results-using-model-1)

[335730.39654 0.006075 84.843161 18.668906]

(generate-virtual-experimental-results-using-model-1)

[-5311.874034 20137.425728 418.947872 -6.874273]





(generate-virtual-experimental-results-using-model-1)

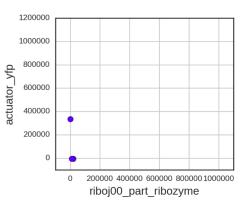
[335730.39654 0.006075 84.843161 18.668906]

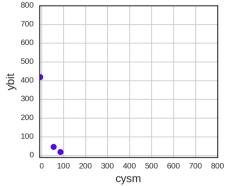
(generate-virtual-experimental-results-using-model-1)

[-5311.874034 20137.425728 418.947872 -6.874273]

(generate-virtual-experimental-results-using-model-1)

[-3967.569575 10886.226517 54.636702 46.125753]





(generate-virtual-experimental-results-using-model-1)

[335730.39654 0.006075 84.843161 18.668906]

(generate-virtual-experimental-results-using-model-1)

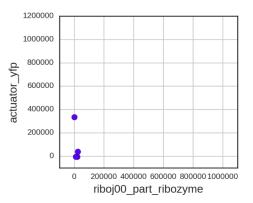
[-5311.874034 20137.425728 418.947872 -6.874273]

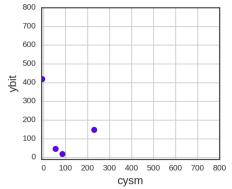
(generate-virtual-experimental-results-using-model-1)

[-3967.569575 10886.226517 54.636702 46.125753]

(generate-virtual-experimental-results-using-model-1)

[38040.924380 23131.858116 230.307509 147.73948]





(generate-virtual-experimental-results-using-model-1)

[335730.39654 0.006075 84.843161 18.668906]

(generate-virtual-experimental-results-using-model-1)

[-5311.874034 20137.425728 418.947872 -6.874273]

(generate-virtual-experimental-results-using-model-1)

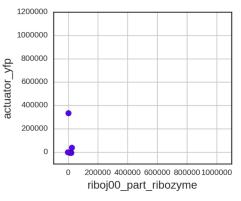
[-3967.569575 10886.226517 54.636702 46.125753]

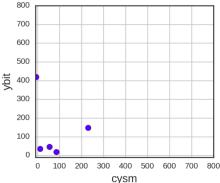
(generate-virtual-experimental-results-using-model-1)

[38040.924380 23131.858116 230.307509 147.73948]

(generate-virtual-experimental-results-using-model-1)

[909.331470 -2293.825225 10.919185 36.128689]





(generate-virtual-experimental-results-using-model-1)

[335730.39654 0.006075 84.843161 18.668906]

(generate-virtual-experimental-results-using-model-1)

[-5311.874034 20137.425728 418.947872 -6.874273]

(generate-virtual-experimental-results-using-model-1)

[-3967.569575 10886.226517 54.636702 46.125753]

(generate-virtual-experimental-results-using-model-1)

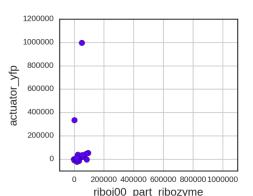
[38040.924380 23131.858116 230.307509 147.73948]

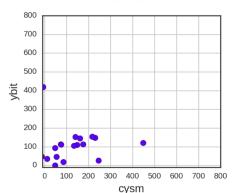
(generate-virtual-experimental-results-using-model-1)

[909.331470 -2293.825225 10.919185 36.128689]

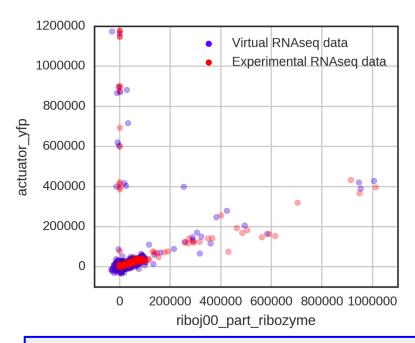
(generate-virtual-experimental-results-using-model-1)

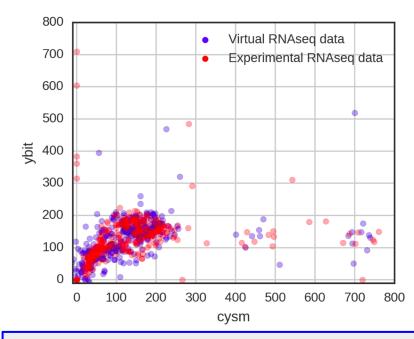
[53525.121077 93310.599669 47.987178 1.289953]





### Compare virtual and experimental RNAseq data





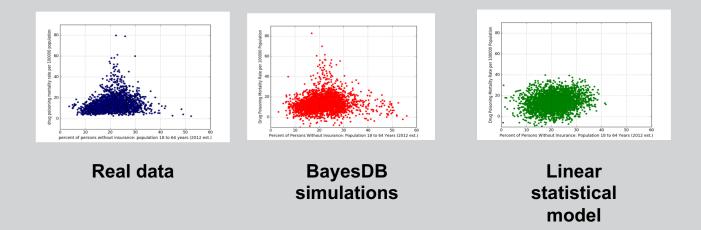
%%bql
SIMULATE cysm, ybit FROM data;

%%bql
SELECT cysm, ybit FROM data;

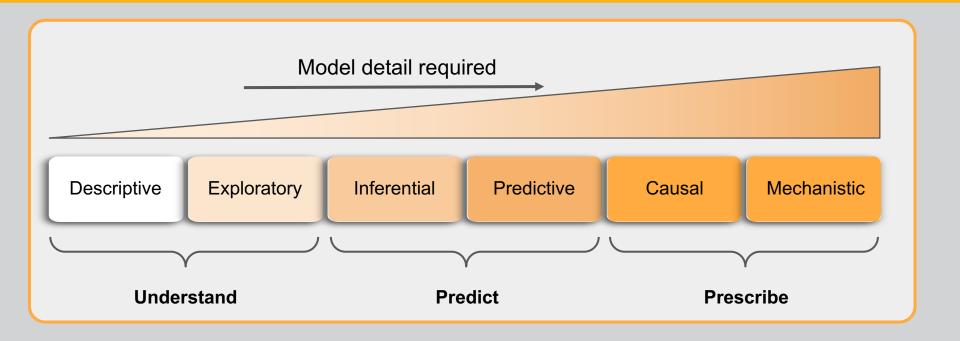
### What is BayesDB?

**BayesDB**: An open-source probabilistic programming platform with built-in automatic model discovery.

BayesDB users can use an SQL-like language to solve data analysis and statistical inference problems in seconds/minutes that otherwise take hours/days for someone with PhD-level expertise.



### What kinds of analysis can BayesDB perform?



NOTE: BayesDB is a research prototype, but we are currently selecting industry and government partners for a new open-source version under development

#### America's socio-political reality



#### Data: empirical state of the nation

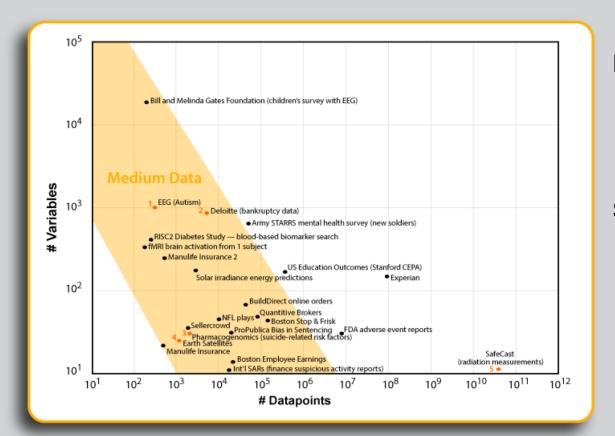
			Datai ompirioai						
id	geo_fips	state	NAME	state_cd_slug	updated	nyt_rating	character	alex	alex_type
4	0101	al	Congressional District 1 (115th Congress), Alabama	al-01	8/6/18 10:38	1) Solid R	Rural/Small To	NULL	NULL
6	0102	al	Congressional District 2 (115th Congress), Alabama	al-02	8/6/18 10:38	1) Solid R	Rural/Small To	NULL	NULL
8	0103	al	Congressional District 3 (115th Congress), Alabama	al-03	8/6/18 10:38	1) Solid R	Rural/Small To	NULL	NULL
10	0104	al	Congressional District 4 (115th Congress), Alabama	al-04	8/6/18 10:38	1) Solid R	Rural/Small To	NULL	NULL
12	0105	al	Congressional District 5 (115th Congress), Alabama	al-05	8/6/18 10:38	1) Solid R	Rural/Small To	NULL	NULL
14	0106	al	Congressional District 6 (115th Congress), Alabama	al-06	8/6/18 10:38	1) Solid R	Mature subur	NULL	NULL
16	0107	al	Congressional District 7 (115th Congress), Alabama	al-07	8/6/18 10:38	7) Solid D	Rural/Small To	NULL	NULL
20	0200	ak	Congressional District (at Large) (115th Congress), Ala	ak-00	8/6/18 10:38	1) Solid R	Rural/Small To	NULL	NULL
24	0401	az	Congressional District 1 (115th Congress), Arizona	az-01	8/6/18 10:38	6) Likely D	Rural/Small To	×	western_ag
26	0402	az	Congressional District 2 (115th Congress), Arizona	az-02	8/6/18 10:38	5) Lean D	Emerging sub	x	diverse
28	0403	az	Congressional District 3 (115th Congress), Arizona	az-03	8/6/18 10:38	7) Solid D	Emerging subu	NULL	NULL
30	0404	az	Congressional District 4 (115th Congress), Arizona	az-04	8/6/18 10:38	1) Solid R	Rural/Small To	NULL	NULL
32	0405	az	Congressional District 5 (115th Congress), Arizona	az-05	8/6/18 10:38	1) Solid R	Mature subur	NULL	NULL
34	0406	az	Congressional District 6 (115th Congress), Arizona	az-06	8/6/18 10:38	2) Likely R	Mature subur	NULL	NULL
36	0407	az	Congressional District 7 (115th Congress), Arizona	az-07	8/6/18 10:38	7) Solid D	Mature subur	NULL	NULL

#### Virtual simulator of the socio-political landscape, as probabilistic program

```
(define data-generating-process-model-0
    (gen []
        (define cluster-id-for-percent_hispanic-percent_asian (categorical [0.27 0.15 0.12 0.11 0.10 0.030.03 0.15]))

(define [percent_hispanic-mean percent_hispanic-std] (cond
        (= cluster-id-for-percent_hispanic-percent_asian 0) [0.153391 0.077936]
        (= cluster-id-for-percent_hispanic-percent_asian 1) [0.030235 0.011154]
        (= cluster-id-for-percent_hispanic-percent_asian 2) [0.130182 0.054384]
        (= cluster-id-for-percent_hispanic-percent_asian 3) [0.067915 0.020329]
        (= cluster-id-for-percent_hispanic-percent_asian 4) [0.437521 0.152850]
        (= cluster-id-for-percent_hispanic-percent_asian 5) [0.719667 0.082805]
        (= cluster-id-for-percent_hispanic-percent_asian 6) [0.237667 0.085933]
        (= cluster-id-for-percent_hispanic-percent_asian 7) [0.175795 0.180930]))
        (define percent_asian-mean percent_asian-std] (cond
        (= cluster-id-for-percent_hispanic-percent_asian 0) [0.035929 0.011853]
        (= cluster-id-for-percent_hispanic-percent_asian 1) [0.011578 0.004625]
```

### **Example applications of BayesDB**



#### Focus on "medium data":

- 100 1M records
- 10 1000 fields

### Sources of "medium data":

- People
- Experiments
- New business processes
- "Big data" reduced down to just what's relevant

# **Outline**

- 1. Motivation
- 2. What is probabilistic programming?

Pedagogical example: simple (or not-so-simple) curve fitting

3. Programmable inference, not just black-box

Application: machine perception via inverse graphics

4. Learning the structure and parameters of probabilistic programs

Application: automatic data modeling for scientific data analysis



5. The MIT Modeling and Inference Stack

### The MIT Modeling and Inference Stack

**Gen**: combining generative models, neural nets, optimization, and Monte Carlo

Perception for robotics

Analyzing scientific images

Research on common-sense Al

BayesDB: SQL-like queries and automatic data modeling

Screening databases for errors and potential anomalies

Searching databases interactively

Detecting predictive relationships from sparse data

Metaprob: lightweight, embedded probabilistic programming in Clojure

Cloudless: containerized deployment and distributed inference

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for info on field testing in 2019

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